Advancing X-ray Science and its Applications

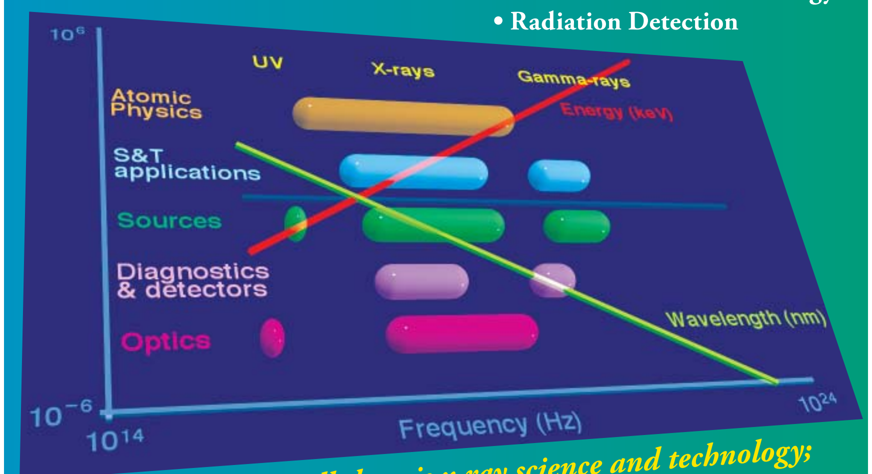
Physics & Advanced Technologies

Physics and Advanced Technologies Directorate
Lawrence Livermore National Laboratory

The Physics and Advanced Technologies (PAT) Directorate at Lawrence Livermore National Laboratory helps ensure the scientific excellence and vitality of the major Laboratory programs through its leadership role in performing basic and applied, multidisciplinary research and development with programmatic impact.

Our R&D spans many areas:

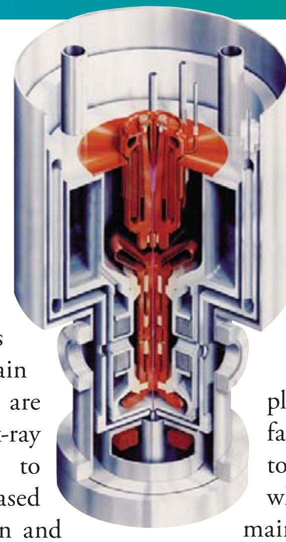
- **Condensed Matter and High Pressure Physics**
- **Plasma Physics and Atomic Physics**
- **Nuclear and Particle Physics**
- **Astronomy and Astrophysics**
- **Accelerator Science and Particle Beam Physics**
- **Optical and Imaging Science**
- **Radiography**
- **Biomedical Science and Technology**
- **Radiation Detection**



Cutting across all these is x-ray science and technology; this brochure describes some of the ways we are advancing x-ray science and its applications.

UCRL-BR-215472

Atomic physics



An impression of the EBIT facility in the Physics and Advanced Technologies Directorate. We use this for detailed atomic physics experiments, including simulating astrophysical phenomena such as cometary x-ray production

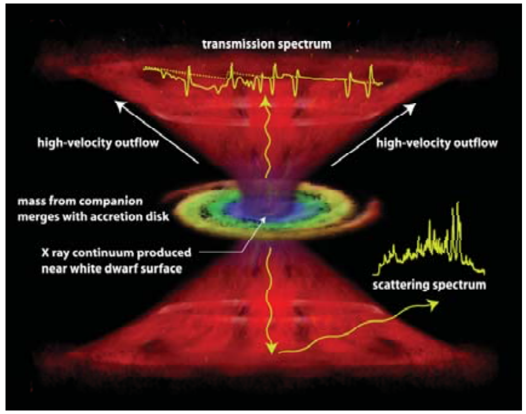
Atomic physics is one of the core disciplines in PAT. Our theoretical and experimental capabilities, together with our collaborators and colleagues inside and outside the Laboratory, are unique and unparalleled elsewhere. One of our responsibilities is to develop, write and maintain codes and databases that are used by the international x-ray community, for example to interpret data from space-based observatories, and to design and interpret experiments at plasma physics facilities. Calculating x-ray transport can be very time consuming; we have just developed a new formulation which is up to a million times more efficient.

Along with theoretical work, we carry out detailed experimental x-ray measurements. High energy density plasmas are studied at our JANUS laser complex, and low energy density plasmas at our spheromak facility and at the DIID tokamak (General Atomics), where we collaborate and maintain an on-site contingent. We also have an Electron Beam Ion Trap (EBIT) that can 'dial up' the plasma parameters we want to study, using it for spectral line identification, and to measure excitation and dielectronic recombination rates. A super-sensitive hard x-ray calorimeter has been added; LLNL is now home to the world's highest resolution and largest area hard x-ray detector.

X-rays for Science: Astrophysics

Our expertise in atomic and nuclear physics, and hydrodynamics, and the outstanding computing capabilities available at LLNL, put us in a great position to simulate and study astrophysical x-ray sources. In one example, we analyze and interpret data from the international x-ray satellite observatories Chandra and the X-ray Multi-Mirror Mission (XMM-Newton). In another, we are studying the effects of active super-massive black

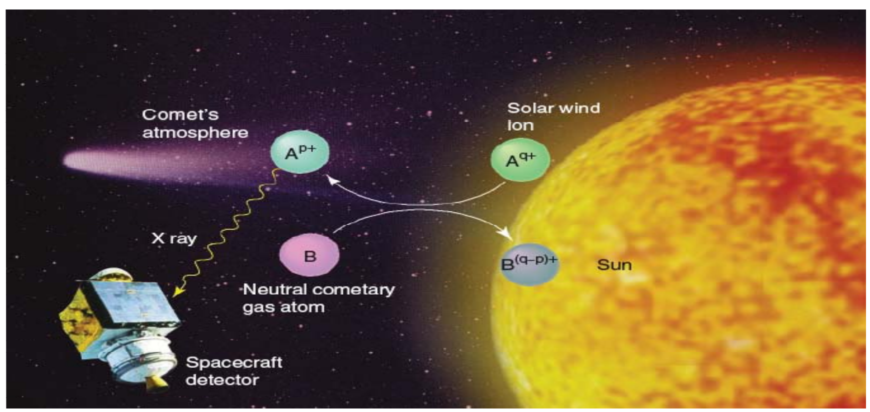
This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.



We are combining detailed atomic and hydrodynamic modeling to interpret x-ray spectra of accretion disk winds. We find that the observed spectra are modified by non-equilibrium opacity in an accelerating ionized medium and depend strongly on the viewing orientation

points for core collapse studies, x-ray burst calculations, and x-ray burst nucleosynthesis. This work provides us an opportunity for many international collaborations.

We play a major role in observational astronomy, in air- and space-born telescope missions. The High Energy Focusing Telescope (HEFT) is a balloon-born experiment that uses depth-graded multilayer optics and Cadmium Zinc Telluride (CZT) pixel detectors to image astrophysical sources in the hard x-ray (20 to 100 keV) band. We did the engineering and shared the development on the optics; low cost fabrication techniques are what make the 72 mirror shells on each of the five telescopes a reality. We use the HEFT detectors for program applications (homeland security). The Nuclear Spectroscopic Telescope Array (NuSTAR), where we hold the Project Scientist role, is HEFT in space. Here we will engineer the optics and also participate in the manufacture. The Energetic X-ray Survey Telescope (EXIST) is a proposed future mission,

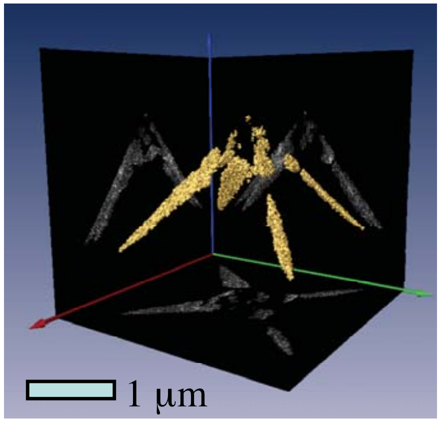


The current explanation for comet x rays is via charge exchange: heavy ions (A^{q+}) from the solar wind flowing from the Sun collide with electrically neutral atoms and molecules (B) in the comet's atmosphere. During a collision, a heavy ion captures one or more electrons from a comet's atmospheric atom, ionizing it to $B^{(q-p)+}$. The solar wind ion, now A^{p+}, momentarily enters an excited state and kicks out an x ray as the electrons return to a low-energy state to image the entire sky each 95 minutes of orbit, detecting extremely faint high energy X-ray sources in an energy range that is poorly explored. We are responsible for instrument design for the Beyond Einstein probe, also known as the Black Hole Finder Probe. Constellation-X is a major (billion dollar class) mission that will fly both soft and hard x-ray telescopes. LLNL is on both the hard x-ray telescope development team and the facility science team.

Our experimental facilities are used for laboratory based x-ray astrophysics experiments. One example is our collaboration with NASA, Columbia University and the University of Missouri-Rolla to explain cometary x-rays. Using the EBIT facility as a surrogate, experiments showed that x-ray emissions form when a continuous stream of charged heavy ions in the solar wind collide with the gases surrounding the nucleus of a comet. The collision neutralizes the solar wind ions, inducing them to give off x-rays characteristic of the ions and gases involved in the collision.

X-rays for Science: Extreme imaging

We want to measure internal properties of matter, from nuclear weapons to viruses. On the large scale, we are developing high-energy tomography systems that have spatial resolutions significantly better than anything currently available, that need specialized computers and image analysis methods. We are developing systems for nuclear weapons stockpile surveillance, cargo container inspection for Homeland Security, spacecraft component certification for NASA, and a wide range of industrial applications. On a smaller scale, we are leading a team to develop x-ray optics for cameras to image mice used in research, with a resolution as small as 10 microns. On the very smallest scale, we are part of a collaboration to use X-ray Free-Electron Lasers (XFEL) to image single molecules, protein complexes, and viruses, with atomic resolution. One challenge is to reconstruct images from continuous diffraction patterns. To do this we have developed a new image reconstruction algorithm that overcomes current limitations. This was used to perform the first truly lensless three-dimensional x-ray imaging. We currently hold the world record for the best spatial resolution.



A 3-D reconstruction of 50 nm gold balls in a pyramid structure using our lensless imaging and new reconstruction algorith. This is being developed for single molecule imaging on future free x-ray lasers.

X-rays for Science: Material properties

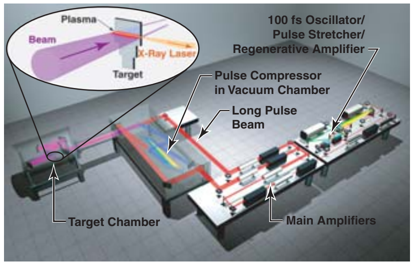
X-rays provide an excellent tool for measuring material properties under extreme conditions, particularly exciting is the now-operational x-ray beamline HPCAT, dedicated to high-pressure studies, at Argonne National Laboratory. We played a major role in its development, investing because it is an enabling capability for our Stockpile Stewardship Program. It will allow us to characterize the structure of high explosives, and low-symmetry phases of plutonium, with unprecedented precision.

We use x-ray spectroscopy and diffraction to measure material properties such as magnetic and structural changes in transition metals and compounds under pressure. X-ray photons are produced at the beamline HP-CAT, part of the Advanced Photon Source synchroton at Argonne National Laboratory

The new research facility will advance high-pressure science by allowing new types of experiments to be performed including measuring the dynamics of electrons, atoms and nuclei and detailed studies of complex materials as functions of pressure, temperature and time. In addition, the new facility will allow a new-generation of high-pressure devices such as large-volume diamond-anvil cells to be used. The ultimate goal is to advance high-pressure synchrotron radiation research and set up a world-leading high-pressure research center accessible to the scientific community at-large. The extension to measuring dynamic properties is one of the reasons PAT is interested in bright, very short pulse x-ray sources.

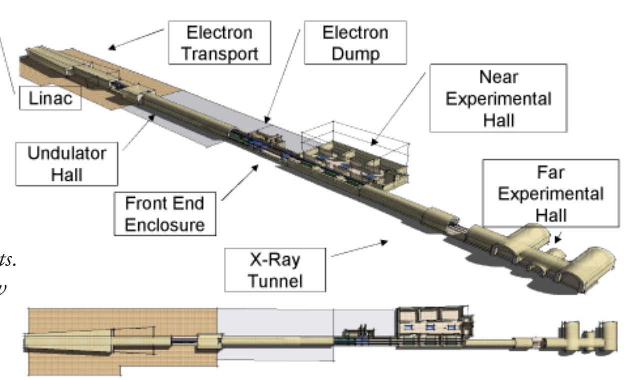
Extreme X-ray sources: X-ray lasers

X-ray light sources are important to us, with combinations of: high brightness, high photon energy (shorter wavelength), short pulse, high repetition rate, and compactness. One scheme is the x-ray laser, dating back back to the 1970's, when scientists realized that laser beams amplified by ions would have much higher energies that beams amplified using gases. In the 1980's, during the time of the Strategic Defense Initiative, x-rays were generated underground at the Nevada Test Site, initiated by nuclear explosions. The first laboratory x-ray laser was demonstrated, at Livermore, in 1984. We are now concentrating on tabletop size soft x-ray systems, ideal for probing and imaging high-density plasmas, and for material science. Our 10 Hz,



Our table-top plasma pumped x-ray lasers are used for basic x-ray laser research, as a diagnostic of high density plasmas, and for materials

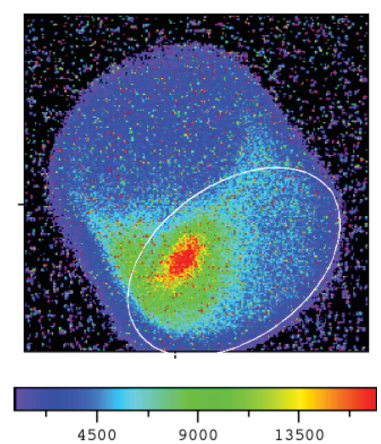
The Linac Coherent Light Source, under construction, will be an x-ray source that is a billion times brighter than existing light sources. We are involved in optics, diagnostics, and experiments. Shown is a facility overview and cross-section.



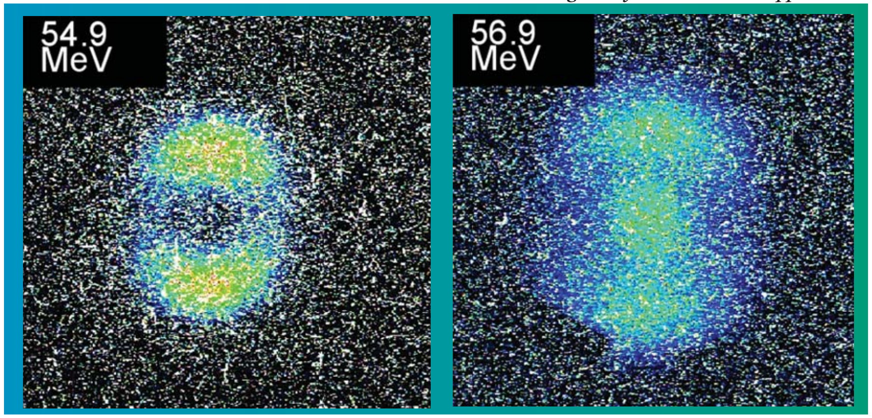
180 Å x-ray laser, pumped by 0.15 J of laser energy per pulse, is in the "water window", ideal for cellular imaging applications. The high repetition rate allows the very short pulses to act as a strobe, providing cleaner images.

For penetrating materials, and obtaining high spatial resolution, shorter wavelength is better. The Linac Coherent Light Source (LCLS is a collaboration between Stanford Linear Accelerator Center, LLNL, Argonne National Laboratory and UCLA, and will be the world's first X-ray Free-Electron Laser (FEL). This will have remarkable x-ray properties: wavelengths of 1 Angstrom and below, pulse lengths into the femtoseconds, and brightness about 9 orders of magnitude larger than current synchrotron x-ray sources. We are responsible for the x-ray transport, optics, and diagnostic systems, and have already prototyped and tested an imaging camera and x-ray optics. Our scientists are leading the teams to perform the plasma and molecular imaging experiments.

Another way of making bright, high-photon-energy x-ray sources is using laser – produced plasmas. A visible laser supersonically heats a volume of target material, which can be a thin foil, a low density doped foam, or a gas. The target becomes a plasma, and radiates in the x-ray region. Using doped low-density foams we demonstrated the highest efficiency x-ray production from solid targets in the 4.7 keV range. Using gas targets we have made sources in the 2-keV, 3-keV, 5-keV, and 13-keV spectral regions. Filling in the gap between 5-keV and 13-keV, and the >13-keV range involves target materials that are initially solid. We use part of the same visible laser that is used to make our high energy density plasmas, so now we have a 'built in' diagnostic ready to use.



Laser energy directed into a Holhraum produces relativistic electrons, which in turn produce x-rays. Here is shown Cu K-alpha fluorescence, x-rays with 8 keV photon energy



Radiographs of a Ta foil taken with our Compton source. By varying the electron energy the x-ray photon energy can be easily change, in thus example to above and below an absorption edge.

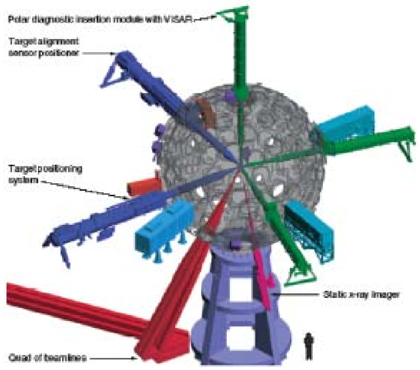
Yet another way to generate x-rays is to scatter visible laser photons off high-energy electrons. The scattering is called Thomson scattering, and the source a Thomson source. We use our 100-MeV electron linear accelerator (linac) and an existing short pulse laser; the resulting x-rays are suitable for radiography, diffraction, and spectroscopy and dynamic characterization of materials. This is now the brightest source for x-ray photon energies above 100 keV. The photon energy is easily tuneable, by changing the voltage on the electron accelerator.

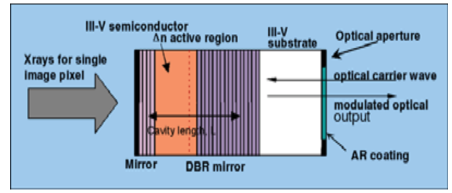
We are now involved in developing this technique, of scattering photons off charged particles for high energy photon – photon scattering, both to make gamma rays and x-rays at the International Linear Collider.

Finally, there is still room to improve 'bremsstrahlung' sources, where fast electron slow down in a solid target and emit bremsstrahlung or braking radiation. They are often used for flash radiography. Our Beam Research Program has developed two technologies to improve them. First is a target that converts electrons to x-rays that can withstand very high doses. Second is a new accelerator wall material and high-current closing switch; together these increase the allowed volts per meter so that much smaller units can be built. There are potential applications to homeland defense and cancer radiation therapy.

Developing diagnostics and detectors: Fast and sensitive x-ray detectors

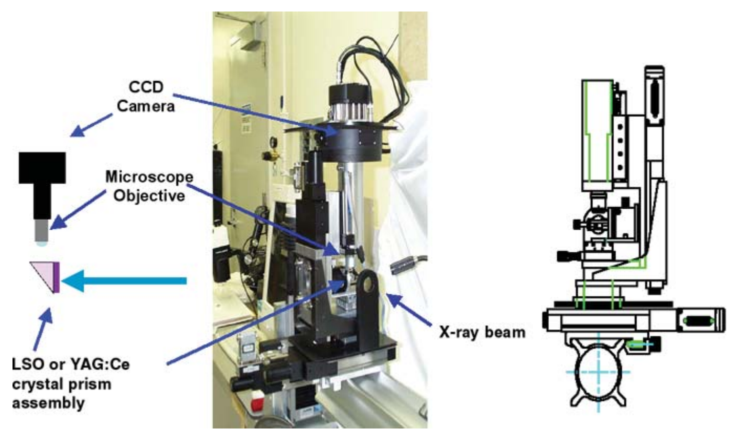
PAT scientists are performing experiments on the National Ignition Facility (NIF) at LLNL, and these need diagnostics. One that we are developing for x-ray detection is both very sensitive (to a single photon) and also very fast. When x-rays are absorbed by a direct band-gap semiconductor, electron-hole pairs are created. The electron-hole pairs create a shift in the





The first quad of beams is shown entering the NIF target chamber, where we are involved in commissioning the diagnostics. Also shown is an expanded view of an individual pixel-vertical cavity radsensor, a concept for a fast, very sensitive imaging x-ray detector that we are developing.

optical absorption spectrum. This is sensed by simultaneously directing an optical carrier beam through the same volume of semiconducting medium that has experienced an x-ray induced modulation in the electron-hole population. At x-ray photon energies greater than 10 keV, we calculate that sub-picosecond temporal responses are possible with single photon sensitivity. Our role in the Free Electron Laser LCLS has driven the development of x-ray cameras. The concept selected uses a small fraction of the beam's light, directly reflected off a thin, polished beryllium foil. Beryllium is chosen because it has a low electron density and tends to absorb few x rays. Beryllium also will be used for many of the reflective optics at the front end of the system where photon densities are highest. When the beam reflects off the foil, it strikes the surface of a 100-micrometer-thick lutetium oxyorthosilicate (LSO) crystal doped with a 5-micrometer-thick scintillating layer of cerium. Visible light is collected by a microscope lens and forms a magnified image on a charge-coupled device (CCD) camera.



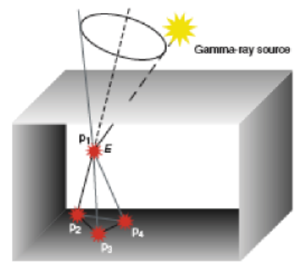
Special diagnostics are needed for the Linac Coherent Light Source, the Free Electron Laser that will be one billion times brighter than existing sources. We have built and tested a camera that can monitor the x-ray beam properties, and withstand the energy deposition.

Developing diagnostics and detectors: Gamma ray imaging

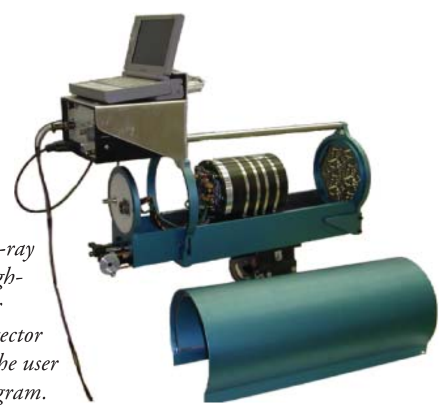
Gamma-rays have the smallest wavelengths and the most energy of any other wave in the electromagnetic spectrum. They are generated by radioactive atoms and in nuclear explosions. Detection of nuclear material, a key need in countering the threat of nuclear terrorism, is possible if gamma rays can be measured at a distance. We have built a prototype, large-size (6400 cm^2) gamma-ray imager based on some existing scintillator crystals. We are also developing a compact gamma-ray imager of high efficiency and spectroscopic resolution using Compton camera concepts; this is also applicable to astronomy.

Superconducting technology and low-temperature techniques are being exploited to provide major advancements in gamma-ray detection; more than ten times improvement in energy resolution has been demonstrated. Mechanical cooling technologies are being used to reduce the weight and power consumption of cooled Germanium detectors while maintaining spectral resolution close to that available using cryogenic fluids. These reductions allow laboratory-quality measurements with a field-rugged detector system consisting of the detector/cooler assembly, a battery pack and a portable computer.

A two-dimensional, segmented germanium detector is one type of Compton camera. In the center is a high-purity germanium crystal. The detector is connected to individual cables and preamplifiers, and the output signals fed into an acquisition system that digitizes and processes the data to extract energies and three-dimensional positions of the gamma-ray interactions.



The Compton camera's omni-directional capability significantly increases gamma-ray sensitivity. A gamma ray enters the detector and interacts through Compton scattering until it is fully stopped by the photoelectric effect. Mathematical algorithms combining all of the gamma rays' energies (E) at each position (p) are used to identify the path of the gamma-ray source.



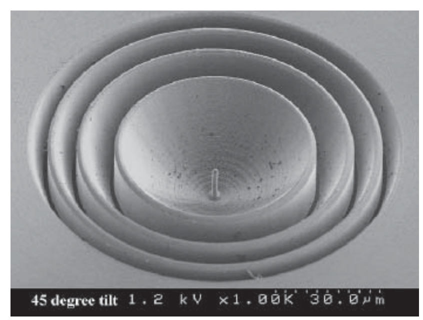
One of our gamma ray detectors, the gamma-ray imaging spectrometer takes pictures of the high-energy gamma radiation given off by nuclear materials. The images are encoded on the detector by using a coded aperture mask that allows the user to recover the image through a computer program.

We are also developing a low-cost, handheld instrument that integrates recent developments in existing commercial cellular telephones with recent breakthroughs in radiation sensor technology. These instruments can be operated manually for communication, location and radiation sensing functions. They can constantly monitor the ambient radiation field and communicate with a central processing system in real time. An analysis algorithm uses information from the entire network to detect, identify and track radiation sources moving through the region. The total volume, weight and power consumption of the hand-held unit is not much larger than the cell phone alone. They would be issued to law enforcement, customs, fire fighters and other security, first-responder and government personnel, to be carried and used as part of their regular, everyday equipment.

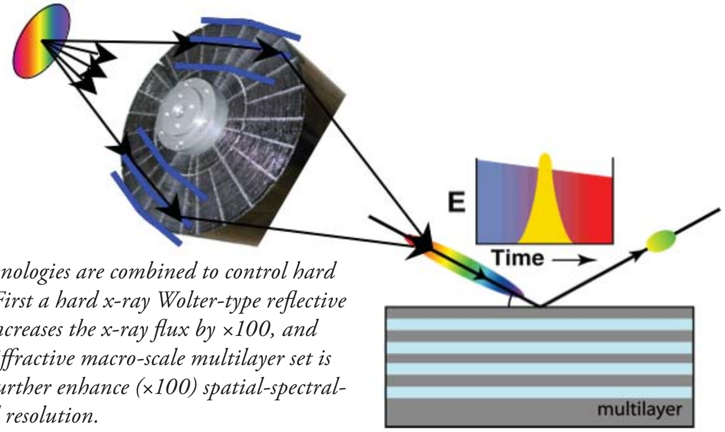
RadNet is a low-cost radiation detector that includes a cellular telephone, a personal digital assistant with Internet access, and a Global Positioning System locator. The basic detector element is also used for astrophysical x-ray detection.

Developing diagnostics and detectors:
Developing x-ray optics

One consequence of our successes in developing high brightness x-ray sources is that we have created another challenge for ourselves: how do we produce optics for reflecting and focusing the beams that last more than a few pulses? To solve this question, PAT scientists have been pursuing a number of ideas. In one, very low Z materials are used, such as beryllium, which are dose-tolerant. Using state of the art engineering facilities at LLNL, we have made and tested low-Z optics with features that are a few microns in size. In another, liquid optics that can be easily



A prototype blazed phase lens made of pure aluminum. The pattern was carved using Livermore's Large Optics Diamond Turning Machine. Each groove is 18.7 micrometers deep, and the final thickness of the disk is 79 micrometers.



Two technologies are combined to control hard x-rays. First a hard x-ray Wolter-type reflective optical increases the x-ray flux by ×100, and then a diffractive macro-scale multilayer set is used to further enhance (×100) spatial-spectral-temporal resolution.

renewed, and whose surface shape can be controlled by electrostatic fields, are being developed.

Focusing very bright x-ray pulses is challenging, and so is manipulating hard x-rays. If we could do this, we would open up a new class of scientific experiments by increasing, by orders of magnitude, the capabilities of the next generation of x-ray sources. To do this we are developing a new generation of x-ray optics, based on hard x-ray (10-200 keV) reflective focusing elements with unprecedented angular resolution. A core optic, which captures and concentrates x-rays across a wide band of energy and input angle, will be combined with diffractive optics based on large scale multilayer structures to further enhance the spatial, spectral and temporal resolving power of the system. Getting the surfaces smooth enough is one of the hardest problems to solve.

We are also helping develop the tools necessary for extreme ultra violet (EUV) lithography, the chosen solution for the next generation of computer chips. We are concentrating on two challenges. First is the development of diffraction-limited optical systems for imaging a mask onto a wafer for use in the lithographic exposure tools. Second is the development of defect-free masks (called reticles) that enable the printing of features with stringent controls on feature fidelity. This program has garnered many awards.

PAT and other LLNL staff have co-developed, with private industry, EUV lithographic equipment and techniques.

X-ray science and technology cuts across all research areas in the Physics and Advanced Technologies Directorate at Lawrence Livermore National Laboratory, from the nanoscale (where we currently hold the word record for three-dimensional reconstruction using our lensless diffraction imaging) to understanding the environment around black holes.

We have current openings for PostDocs in many of the areas discussed above, as well as opportunities for collaborative research.

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